

Modeling pollutant dispersion in urban areas with computational fluid dynamics

by

Benjamin Ishii

B.S., University of Oklahoma, 2010

A REPORT

submitted in partial fulfillment of the requirements for the degree

MASTER OF SCIENCE

Department of Chemical Engineering
College of Engineering

KANSAS STATE UNIVERSITY
Manhattan, Kansas

2019

Approved by:

Major Professor
Dr. Larry Erickson

Copyright

© Benjamin Ishii 2019.

Abstract

Pollution is a major issue for urban areas all around the world. This report reviews the recent literature on modeling and pollution dispersion in urban areas with the application of computation fluid dynamic (CFD) models. A review of atmospheric turbulence and weather conditions is provided as pertaining to dispersion modeling. When applying CFD, the modeler must specify the closure model, which could be direct numerical simulation (DNS), Reynolds average numerical simulation (RANS), or large eddy simulation (LES). A comparison of the RANS and LES models is provided. The main advantages of CFD is that it offers advanced modeling that can account for turbulence under multiple weather conditions and 3-dimensional obstructions in the flow field.

The recent research focuses on how CFD can be used to predict pollution concentrations without measurement devices or physically altering an urban landscape. Multiple researchers have explored pollution dispersion near roadways, specifically modeling pollution emission and the effect of roadway barriers on pollution dispersion. Other research focused on modeling a larger portion of a city where the buildings and street canyons play an important role in the flow patterns (and the effects on pollutant dispersion) within the city. The research explores the possibility of modifying urban areas to allow for increased pollutant dispersion. The recent research shows that CFD is a powerful tool for modeling pollutant dispersion and that more research is required to take full advantage of CFD in this area.

Table of Contents

List of Figures	v
Acknowledgements.....	vi
Chapter 1 - Introduction.....	1
Chapter 2 - Weather Conditions	4
Chapter 3 - Modeling with Computational Fluid Dynamics	9
DNS	9
RANS.....	10
LES	10
Chapter 4 - Comparison of Models.....	12
Chapter 5 - Applications	16
Chapter 6 - Future Study.....	27
Chapter 7 - Conclusion	29
References.....	30

List of Figures

Figure 2-1 Plume Behavior under Various Temperature Lapse Profiles. The Temperature Profile is Shown on the Left and the Plume on the Right. (adapted from Krishna, 2017)	5
Figure 4-1 Comparison of RANS and LES. (Som and Pomraning, 2012)	13
Figure 4-2 Turbulent Kinetic Energy Profile of a Stable Stratification. (adapted from Pontiggia, 2009).	15
Figure 5-1 Modeling results showing the 3 m high horizontal streamlines and CO concentration field with effect of trees in Aveiro. Contours refer to the period between 10 and 11 a.m. Unfilled rectangles indicate trees blocks and the white triangle is the AQS location. (adapted from Amorim et al., 2013)	19
Figure 5-2 Modeling results showing the 3 m high horizontal streamlines and CO concentration field without the effect of trees in Aveiro. Contours refer to the period between 10 and 11 a.m. Unfilled rectangles indicate trees blocks and the white triangle is the AQS location. (adapted from Amorim et al., 2013)	20
Figure 5-3 Top - Surface temperature in Celcius at 9:00 hours. Bottom - NO concentration (ppm) at 9:00 hours. (adapted from Huang et al., 2008)	23
Figure 5-4 Top - Surface temperature in Celcius at 11:00 hours. Bottom - NO concentration (ppm) at 11:00 hours. (adapted from Huang et al., 2008).....	24
Figure 5-5 Physical scale model of the Pâquis city landscape, where the green indicates emission of SF ₆ and the blue arrows represent the air flow. (adapted from Triscone et al., 2016).....	25
Figure 5-6 Top - wind speed as a function the height z. Bottom - measurements of dimensionless gas concentration. (adapted from Triscone et al., 2016).....	26

Acknowledgements

I am grateful to Dr. Larry Erickson for providing guidance and support throughout the composition of this report. A special thanks to Dr. James Edgar, Dr. Jennifer Anthony, and Dr Mingjun Wei for being on my supervisory committee.

I am grateful to Quest Consultants for providing the opportunity to work and pursue an advanced education. Thank you to all those at Kansas State University who worked to provide distance education to me and many others.

I could not do this without my family who loved and supported me while I worked my way through five years of graduate school. I am deeply grateful to my wife for her support and encouragement.

Chapter 1 - Introduction

Pollution has a major impact on human health. Many studies have researched the physiological impacts of pollution. The consensus of the research is that pollution negatively impacts human health. Due to human activity in urban areas, pollution concentration is often high in these densely populated areas. The UN reports that 55% of the global population lives in urban areas as of 2018, and projects that this number will increase to 68% by 2050 (United Nations, 2018). Thus, the study of pollution dispersion in urban areas is a growing topic of concern.

In 2007, Pope reviewed the current state of research on particulate air pollution and human health. The paper by Pope concludes that both concentration and exposure duration have a strong correlation with the persistence and potency of adverse health effects (Pope, 2007). In 2011, R  ckerl et al. updated the review of physiological impacts with more recent studies. The conclusion of this body of work shows that air pollution is causing many health issues in both adults and children (R  ckerl et al., 2011). Some conclusions of this work are listed below.

- There is strong evidence and agreement in the research that particulate pollution is connected to cardiovascular disease that may result in hospitalization and in some cases death.
- Most studies found pollution had an adverse impact on respiratory disease, including lung cancer.
- There is some evidence for increased inflammation due to pollution.
- There is some evidence for adverse reproduction and prenatal outcomes.
- New research suggests pollution may have neurotoxic effects.

All these consequences combined paint a dismal picture of the impact of pollution on humans. More importantly the consequence highlights the importance and urgency of the study of air pollution. Research continues in this area and is especially needed to isolate the physiological impacts in relation to specific pollutants. With a world where industrialization is spreading and urban areas are growing, pollution will continue to be a human health problem for the foreseeable future.

Measuring pollution concentration is an important part of studying pollution, but measurement devices have their limitations. Pollution most often refers to a mixture of many pollutants. Some of the categories that allow for more specificity are: particulate matter (PM), ultrafine particles (UFP), SO₂, NO_x, CO, CO₂, O₃, and black carbon. Measurement devices can be fitted with sensors to measure the concentration of one or possibly more specific pollutants, but typically these devices get more expensive with increased sensing ability. In addition, measurement devices can only measure concentration at a single point at a single time. This applies to both stationary and portable devices, both of which have their benefits and disadvantages. Placing tens or hundreds of measurement devices necessary to measure pollution in a large area or even a significant portion of a city may be cost-prohibitive. With respect to cities, the measurements may only be useful for a short time period due to the dynamic nature of cities with pollutant emissions and city landscapes changing constantly. Thus, it may not be practical or economically feasible to measure the many components of pollution, or measure pollution over a large area with a significant density of coverage.

Pollutant measurement devices allow researchers to gather data about pollution concentrations; and this data can be used to develop advanced models of pollution dispersion. Field data is important for validating dispersion models for pollution dispersion applications.

Computational fluid dynamics (CFD) allows the transient behavior of pollution dispersion to be modeled in a 3-dimensional space. These types of models offer researchers a practical way to simulate multiple pollutants and model pollutant concentrations in a city or a portion of a city. CFD offers the possibility of predicting changes in pollutant concentrations due to proposed changes to a city landscape before any construction takes place. This capability may allow city planners to simulate multiple layouts and ultimately improve the dispersion of pollutants in the city or area.

Due to the cost of measuring pollutants throughout a large area and the limitations of measurement devices, computer modeling is a practical way to study pollutant concentrations within urban areas. The purpose of this paper is to investigate the use of CFD modeling of pollutant dispersion in urban areas. Modeling pollution dispersion involves modeling the flow patterns and turbulence associated with local weather conditions. A 3-dimensional model is required to model the buildings, roads, vehicles, and vegetation that make up a city landscape. CFD can account for both weather conditions and large obstructions to model pollutant dispersion. Thus, CFD is a significant tool in the research of pollutant dispersion in urban areas.

Chapter 2 - Weather Conditions

The atmospheric boundary layer (ABL), also known as the planetary boundary layer, is the portion of the troposphere that is dominated by interactions between the atmosphere and the surface. While there is not an exact height defined for the ABL, it is commonly understood to be within the first kilometer of the troposphere. The stratosphere and the portion of the troposphere above the ABL are usually not of interest, except in the study of long distance pollutant travel (Pasquill and Smith, 1983). Examples of some of the types of long-distance pollutants include: volcanic dust, radioactive material, and industrial pollutants. But for this paper, the topics discussed will be confined to the ABL.

Atmospheric stability is extremely important when modeling the dispersion effects of wind. Atmospheric stability is the ability or inability to resist vertical movement in the atmosphere. The vertical movement of air is of particular interest in determining the dispersion of pollutants. The level of stability is dependent upon the temperature lapse rate, where lapse rate is the change in temperature with respect to elevation (Finlayson and Pitts, 2000). As a portion of the air rises in the atmosphere, it expands and cools; if a portion of air cools faster than the lapse rate, then it begins to fall. This scenario describes a stable system, or a system that resists vertical movement. If the same portion of air cools slower than the lapse rate, then it is warmer than surrounding air and continues to rise. This scenario describes an unstable system. An important factor in the heating and cooling of air is the moisture in the air. Thus, stability is a function of humidity and temperature lapse rate. The atmospheric stability and wind speed can be used to describe the turbulence of the atmosphere (Foken, 2017). Figure 2-1 illustrates different plume behavior depending on the lapse rate or potential temperature. Part A) presents

an unstable atmosphere, part B) presents a neutral atmosphere, and part C) presents a stable atmosphere.

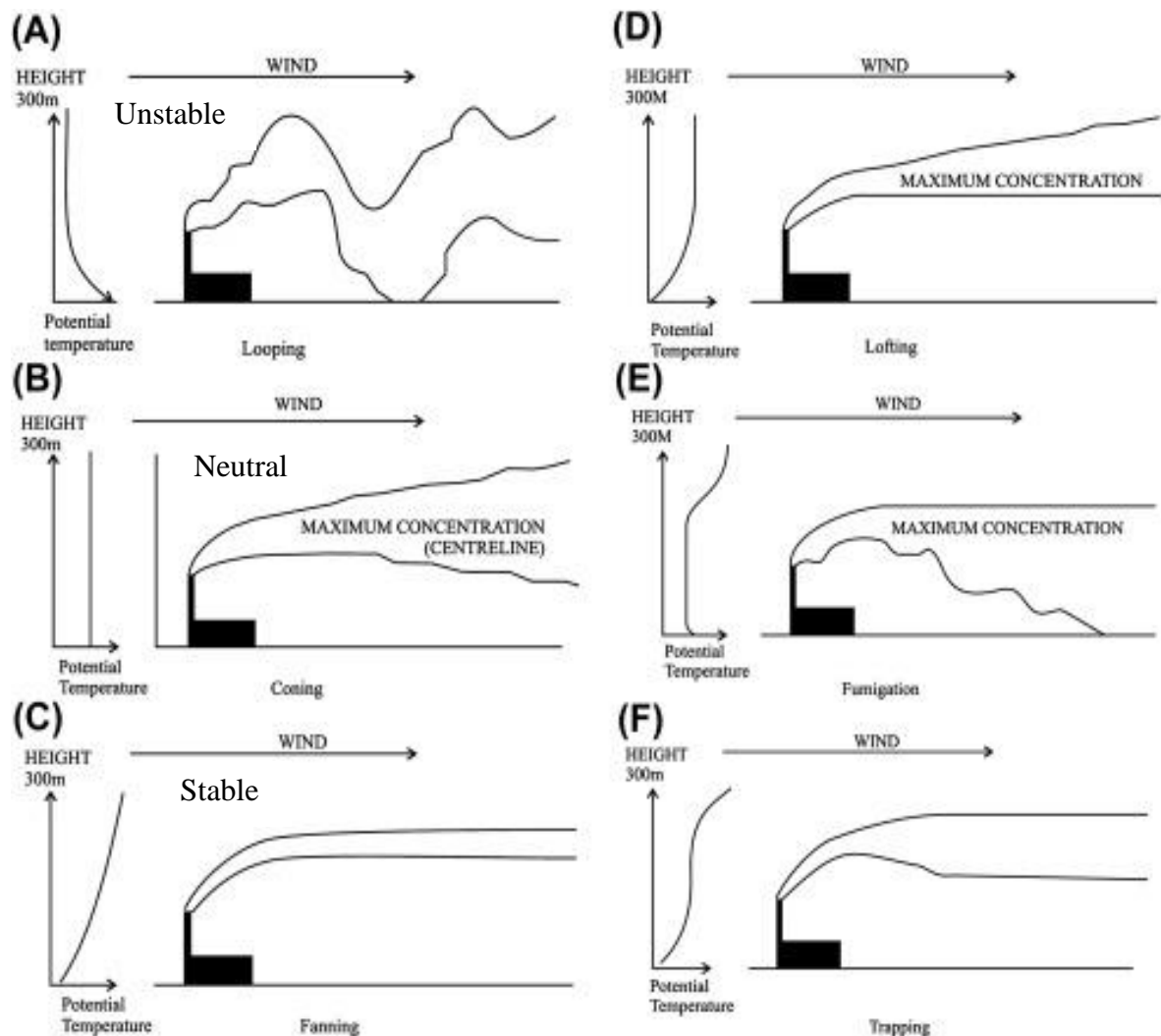


Figure 2-1 Plume Behavior under Various Temperature Lapse Profiles. The Temperature Profile is Shown on the Left and the Plume on the Right. (adapted from Krishna, 2017)

All air quality models must account for mixing in both the lateral and vertical planes. The amount of mixing is related to the degree of turbulence, which in turn is related to the atmospheric stability. Air quality models typically classify stability and relate the classification to turbulence, or equate turbulence as a continuous function of stability parameters. There are a number of methods of classifying atmospheric stability. Some of the most popular methods are

Pasquill Gifford Turner (PGT), Richardson number, and Monin-Obukhov length (Pasquill and Smith, 1983). These methods may be used directly or indirectly to determine parameters for lateral and vertical dispersion. In addition, these methods combined with the wind speed can be used to estimate the vertical velocity profile of the air.

Another weather phenomenon related to atmospheric stability is inversion. An inversion is a significant deviation in the change in properties of the atmosphere from one elevation to another elevation. Inversions are often associated with changes in the lapse rate, where the slope of the lapse rate changes from positive to negative, or vice-versa. The conditions above and below an inversion can differ greatly, even to the point where the wind can be blowing in opposite directions. Figure 2-1 illustrates inversions: a plume dispersing above an inversion in part D), a plume dispersing below an inversion in part E), and a plume dispersing between two inversions in part F).

The weather data used in recreating and predicting pollution dispersion ultimately is gathered from weather stations equipped with weather sensors and measurement devices. The weather data collected from existing weather stations, that gather and store hourly weather data throughout the year, are insufficient to fully and accurately recreate the conditions in models, such as CFD. Many weather stations gather a limited set of data that only allows the estimating of a wind speed profile, atmospheric stability, and vertical turbulence. Working with limited measurements is possible, but it often involves a generalization of the diverse weather conditions.

The weather stations that make up the United States national weather system are limited in data collection. The wind speed and direction is measured at 10 meters from grade (WMO, 2017) at airport weather stations. Although not as common, wind speeds can be measured at

other heights. For example, the United States Climate Reference Network (USCRN) collects wind speed and direction at 1.5 meters from grade (NCEI, 2019). (Note that the devices in this network are also required to measure temperature in the air and surface temperature.) While wind speed measurement heights may vary from station to station, typically these measurements are limited to one elevation. If wind speed measurements were taken at multiple elevations, they would allow better characterization of the vertical wind speed profile. Wind speed is measured with anemometers; and these instruments vary in type, measurement technique, and precision. Typically, an anemometer is combined with another device to determine the direction of the wind. One type of anemometer, an ultrasonic anemometer, can be coupled together with other anemometers to produce a 2-dimensional and even 3-dimensional measurements of wind velocity. Typically, measurements are 2-dimensional, accounting for the speed and the direction in the horizontal plane. Vertical air movement is often neglected because the devices required for these types of measurements are rarely found on typical weather stations. Vertical air movement, if measured, would provide data that directly relates to atmospheric stability.

Stability is an important part of modeling dispersion in the atmosphere because it has a significant impact on the rate of dispersion. Depending on the application, it may be important for the model inputs to reflect local conditions. In such a case, the modeler would either rely on historical weather data or gather the data independently. It is important to understand the weather measurements and how these can be used in the inputs to CFD models. Research on commercially available stability monitors has shown that radon measurement devices can be correlated with stability. The researchers correlated atmospheric stability with pollution measurements to show that pollution concentrations were highest during stable weather conditions (Chambers et al., 2015).

Extreme weather can be difficult to accurately measure. In most extreme weather there is increased turbulence and hence increased dispersion. Examples of extreme weather include:

- Heavy rain
- Hail
- Blizzards
- Tornadoes
- Hurricanes

Hurricanes and tornadoes are examples of extreme weather with high wind speeds. In these cases, the increased wind speeds will increase the rate of dispersion. Heavy rain, hail or snow all have liquid or solids falling through the air. These scenarios have increased vertical movement resulting in increased vertical dispersion. In the case of precipitation, the falling precipitation removes pollutants from the air resulting in decreased pollutant concentrations. Therefore, the extreme weather scenarios considered above increase the amount of mixing and decrease the dispersing concentrations. The exception to this may be long-distance transport of pollution, where there are effects of extreme weather on the stratosphere and upper troposphere, which are not addressed in this paper.

Chapter 3 - Modeling with Computational Fluid Dynamics

Computation fluid dynamics (CFD) provides a sophisticated tool to account for turbulence in dispersion modeling. While the goal of CFD is to recreate realistic phenomena, CFD can only provide an estimate, where the accuracy and precision depend on the implementation. CFD ultimately seeks to solve the Navier-Stokes equations. There are three sets of equations: 1) conservation of mass, 2) conservation of momentum, and 3) conservation of energy. Currently, there is no known analytical solution to the full set of Navier-Stokes equations without simplification. Because of this, multiple strategies have been employed to make CFD more accessible, namely: DNS, RANS, and LES. With any approach to CFD the domain and grid must be sized appropriately. The domain should be larger than the largest turbulent eddy and the grid size should not exceed the Kolmogorov scale. The Kolmogorov length scale is defined as:

$$\eta = \left(\frac{\nu^3}{\epsilon} \right)^{1/4}$$

where ν is kinematic viscosity and ϵ is the rate of dissipation of turbulence kinetic energy (Wyngaard, 2010).

DNS

One approach is direct Navier-Stokes (DNS); this approach solves the Navier-Stokes equations without any approximation of the turbulence. (Coleman and Sandberg, 2010). The drawback to this approach is that the all eddies, from the largest to the Kolmogorov scale, must be resolved. The DNS approach is resource intensive and may not be feasible for many of the applications related to pollution dispersion.

All other approaches seek to modify the equation, such that computers can solve the equations faster and/or more efficiently. Note that any modification to the Navier-Stokes equations is connected to a set of underlying assumptions. These assumptions are important in understanding the limitations of the model.

RANS

Another approach is the Reynolds averaged Navier Stokes (RANS) model. This employs Reynolds decomposition to transform velocity, pressure, density, etc. into a time-averaged value and a turbulent fluctuation term (Tabatabaian, 2015). The RANS model requires a turbulence sub model to estimate or specify the turbulence fluctuation term (Gatski et al., 1996). One common turbulence sub-model is the k-epsilon model, where k is the turbulent kinetic energy and epsilon is the dissipation rate. (Launder and Spalding, 1974). All of the known turbulence sub-models are limited in describing turbulence and have not been successful in fully reproducing turbulent flows. The RANS approach provides increased computational performance due to the turbulence sub model that allows the simplified equations to be analytically solved. However, it lacks a description of the eddies and isotropy at small scales. Another common issue with RANS is the dissipation of turbulence. Batt et al. showed that the turbulence in the wind, modeled with RANS, dissipated significantly over a one kilometer domain (Batt et al., 2018).

LES

The large eddy simulation (LES) model also attempts to increase CFD computing speeds. The model is based on the idea that at some small scale the eddies can be approximated universally, while larger eddies dominate mass, momentum, and energy transport (Steffens et al., 2013). In order to solve the large scale eddies, first a filter is applied. Ferziger identifies three

types of filtering: Gaussian, box, and cutoff (Gatski et al., 1996). Based on the grid, the Reynolds stresses are modeled accounting for:

- Interactions between large scale eddies that produce small scale eddies
- Interactions between large and small scale eddies
- Interactions between small scale eddies that produce large scale eddies

The LES model is under the same constraint as DNS for domain size to be large enough to capture the largest turbulent eddies. But LES can have a larger grid size compared to DNS, as it does not have to capture the small-scale turbulence. Overall, LES provides a balance between the resource intensive DNS model and the less precise RANS model.

Chapter 4 - Comparison of Models

The choice between DNS, RANS, and LES is left up to the modeler; based on the specific problem and the available computational resources. A comparison between the commonly used RANS and LES illustrates some of the reasons a modeler may choose one over the other. The differences between RANS and LES are illustrated in the modeling of diesel spray as shown in Figure 4-1. Although the content does not directly relate to the topic of this paper, the comparison of RANS and LES is applicable to CFD models in general. This figure shows two columns, where each image is a temperature heat map of a diesel spray at four different snapshots of time, under engine conditions, generated from the CFD modeling results (Som and Pomraning, 2012). The left and right column presents a reproduction of the experiment with a RANS model and LES model, respectively. The results of the RANS model demonstrates the characteristic even mixing without eddies. The LES results shows how the model accounts for eddies, but not the small-scale eddies. In this case the resources required for these models cannot be compared because the authors did not indicate the computational resources and overall times. Depending on the application, especially considering the size of the grid and resolution of the mesh, a faster computational time may be a determining factor. Typically, LES is computationally more intensive than RANS.

Steffens et al. (2013) studied these differences by modeling dispersion around a roadside barrier with both RANS and LES. Both of these models were available through the use of the comprehensive turbulent aerosol dynamics and gas chemistry (CTAG) model; which was developed by the Energy and Environmental Research Laboratory (EERL) at Cornell University. CTAG employs ANSYS Fluent, a commercial software package, for the CFD flow solver. Previous work evaluated air pollutant dispersion near roadside barriers for only one atmospheric

stability. This work attempted to evaluate the same scenario under multiple atmospheric stabilities with both RANS and LES. The simulations were compared to experiments performed where sulfur hexafluoride was released upwind of a barrier, where the barrier dimensions were 90 meters long with a height of 6 meters. Concentrations were measured downwind on the opposite side of the barrier and meteorological conditions were recorded. The study found that while both models captured the overall trend, that LES performed better than RANS. In addition the authors showed that multiple stabilities could be accounted for in both RANS and LES. The LES model is more appropriate for modeling flow around complex geometries and RANS may be appropriate for simple geometries.

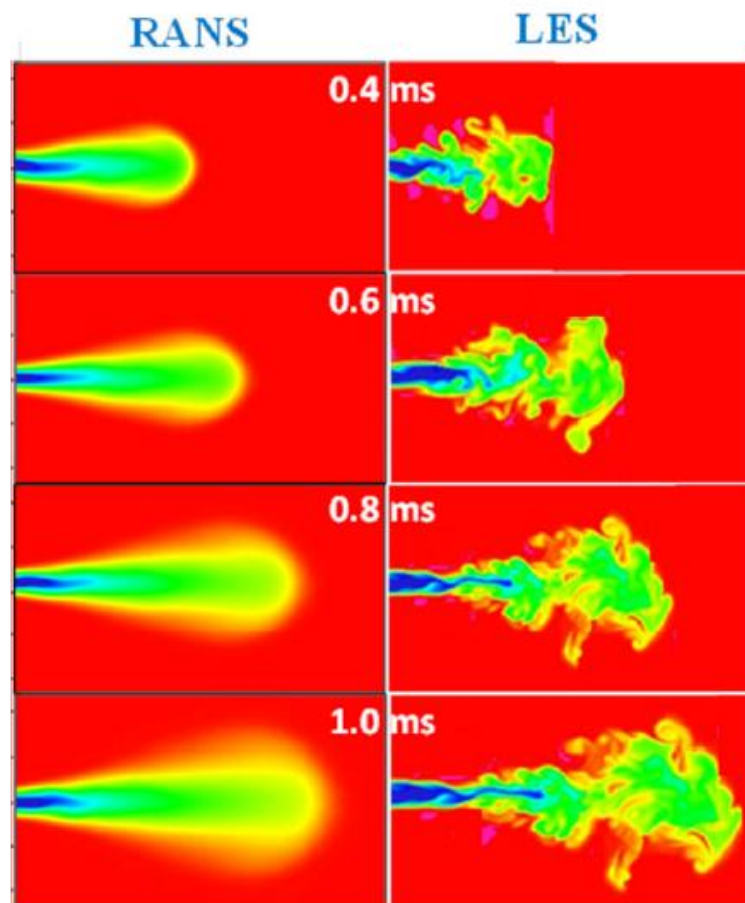


Figure 4-1 Comparison of RANS and LES. (Som and Pomraning, 2012)

The closure model, used with the RANS model, can be combined with or modified to account for stability parameters. The oft used k-epsilon closure model can be related to stability due to the turbulence description. One example of this, is a paper that showed k-epsilon parameters can be modified based on Monin-Obukhov similarity theory to model a stable and natural stability (Pontiggia et al., 2009). Figure 4-2 presents a comparison of results for the turbulent kinetic energy vertical profile of Monin-Obukhov, standard k-epsilon, and a modified k-epsilon models. These results show that the standard k-epsilon model deviates from Monin-Obukhov similarity theory, but can be modified to closely resemble the expected profile.

The LES model accounts for stability differently than the RANS model. One research modeled stability by altering the subgrid-scale model and its parameters (Basu and Porte-Agel, 2006). The model allowed dynamically generated parameters based on the stability and filter-scale. These results compared favorably with field observations, but the model was not tested with large-scale dispersion experiments. The authors recognized the need for further study in modeling very stable conditions.

The RANS model is attractive for its computational efficiency when compared to LES. But the RANS model lacks the detail and resolution of eddies that LES offers. When the bulk flow or average pollution concentrations are sufficient, then RANS is a better fit. On the other hand, LES should be used when capturing the detail of the flow patterns is important. In addition, common sub-models for RANS, like k-epsilon, do not differentiate lateral and vertical mixing rates. Thus, LES is typically a better fit for modeling atmospheres that are unstable.

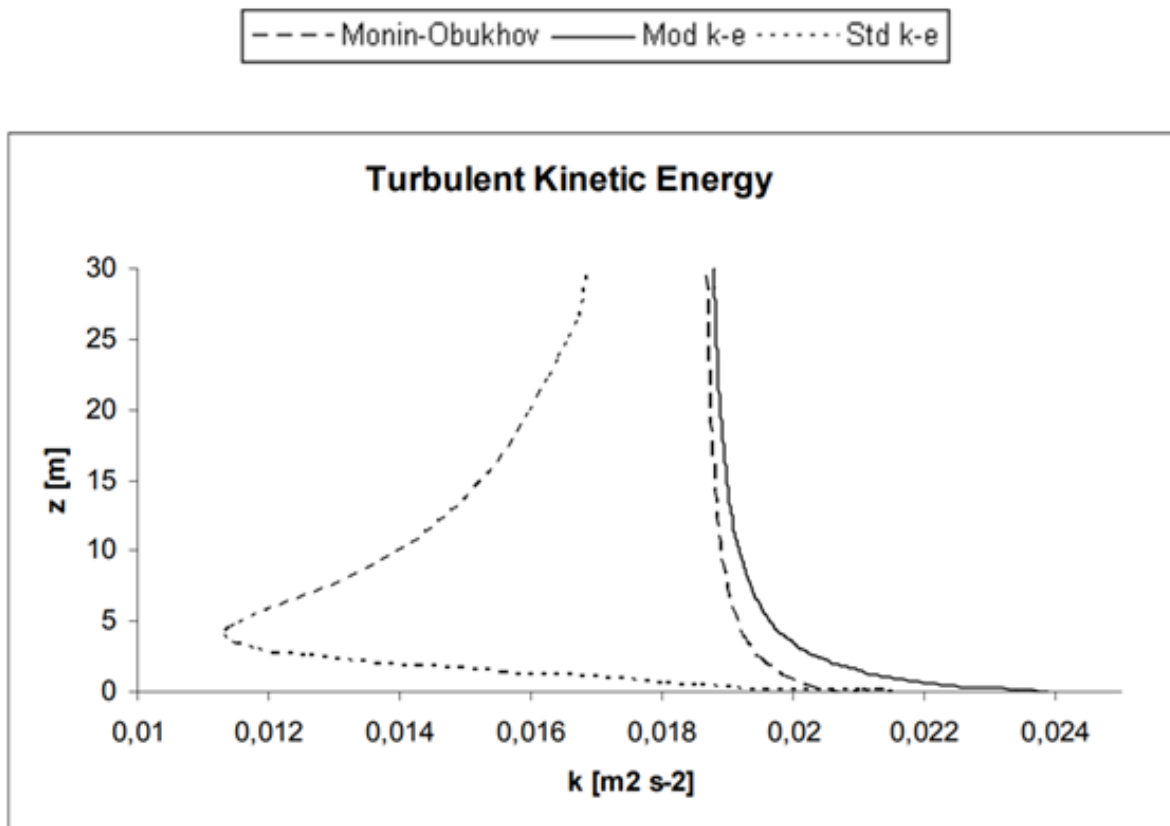


Figure 4-2 Turbulent Kinetic Energy Profile of a Stable Stratification. (adapted from Pontiggia, 2009).

Chapter 5 - Applications

Much of the recent research regarding CFD and pollution focus on dispersion in city landscapes. Modeling pollution in 3-dimensions in CFD for a city, allows researchers to predict pollutant concentrations without expending the resources to cover a large area with measurement devices. This type of model could also be coupled with local weather measurements to determine which weather conditions result in “too high” pollution concentrations. Many of the studies explore the idea of predicting pollution dispersion in a city or a part of a city using CFD models. These types of predictive studies allow modifications or additions to cities to reduce the impact of pollution on highly populated areas.

Steffens et al. studied a number of roadway configurations (Steffens et al., 2014). They included elevated roads, depressed roads, roads with a single barrier, and roads with barriers on both sides. In this set of simulations, the authors reported difficulty simulating vehicle induced turbulence by modeling vehicles, instead they accounted for vehicles by artificially adding turbulence to the model. These studies showed that effective barriers decreased the pollutant concentrations downwind, but increased the concentrations on the roadway. Another set of experiments by Steffens et al. looked at vegetation barriers along roadways (Steffens et al., 2012). The study compared field measurements with a CFD model of a roadway lined with trees. The field measurements captured particulate concentration and particulate size at two different elevations. The CFD model accounted for the flow obstructions, particle deposition, and particle coagulation. The study found that the CFD model underpredicts concentrations of particles smaller than 50 nm compared to the field measurements. This paper shows the difficulty in modeling a range of particle sizes and the interactions with complex geometries,

such as vegetation. This paper did not include areas with traffic signals, but the stop and go that occurs at traffic signals can impact pollution emissions and dispersion (Kwak et al., 2018).

Chang and Meroney compared wind tunnel modeling experiments to calculations performed with RANS and LES models (Chang and Meroney, 2003). The authors varied turbulence models, boundary conditions, and grid resolution to best model the wind tunnel experiments. The wind tunnel experiments employed 1:50 scale models of buildings to study urban street canyons. The authors gathered visualizations of the flow and tracer gas concentrations. The scale model wind tunnel tests revealed that changes to the geometry, such as distance between buildings, can significantly change the flow patterns. The modeling revealed that the air flow and eddies formed around the sharp edges of the walls are important to model in order to capture the pollutant concentrations close to walls. Based on this observation, it is no surprise that the results showed that the LES model reproduced the wind tunnel data more accurately than the RANS model. In this study, the quantitative comparison was based solely on concentration measurements. There were no measurements of velocity. And the authors did not compare the flow patterns from the scale model with the CFD models. The authors did not address atmospheric stability or temperature gradients because they limited the study to a wind tunnel, which most likely generated a flat wind speed profile.

A study by Amorim et al. (Amorim et al., 2013) studied the “impact of urban trees over the dispersion of carbon monoxide (CO) emitted by road traffic, due to the induced modification of the wind flow characteristics.” In this study a RANS model was applied with a k-epsilon closure. The k-epsilon closure was modified to account for trees with inputs such as porosity and leaf area density. Vehicle emissions were modeled as line source assuming a constant release rate based on vehicle traffic data. The interactions of the vehicles with the wind field

were neglected. The study also neglected any chemical reactions with CO. The modeling consisted of two areas, one in Lisbon and one in Aveiro. Both urban areas included at least one street lined on both sides with mature trees. The CFD model was set up to simulate these areas as-is (with trees) and without the trees. The study concluded that the trees decreased the CO concentration below roof-level by 16% on average and increased the concentration above the roof-level. This was attributed to the differences in flow patterns caused by trees lining the street versus no trees. The results showed good agreement with measurements of CO collected from the Portuguese air quality system (AQS) monitoring station. The CO measurements were only collected at one location in each of the chosen areas. The conclusions of this paper are only supported by the modeling. An additional study would be needed to confirm the conclusions by measuring pollutant concentrations above and below roof levels in an urban area before and after planting trees. Another improvement could be adding additional sensors especially CO monitors and wind speed measurements at separate elevations. In addition, the authors failed to evaluate the model over a range of atmospheric stabilities.

Zheng et al. modeled an area of Shenyang, China with advanced weather modeling (Zheng et al., 2015). A mesoscale model was used to simulate the wind and turbulence in a large area on the order of tens to hundreds of kilometers. The authors then coupled the large-scale weather model with a RANS CFD model. Weather data was collected from approximately 17 different weather stations during winter and summer seasons. The CFD model consisted of a 600 meter by 600 meter area with large buildings. The mesoscale model predicted temperature and wind speed profiles. The CFD model introduced pollution into the model as a point source. The paper showed that complicated wind patterns could be developed by coupling a mesoscale weather model with a CFD model to simulate pollution dispersion. The mesoscale model

closely replicated the wind speed and temperatures during summer, but deviated compared to winter measurements. The authors suggest that the model is more sensitive to heat additions in the winter.

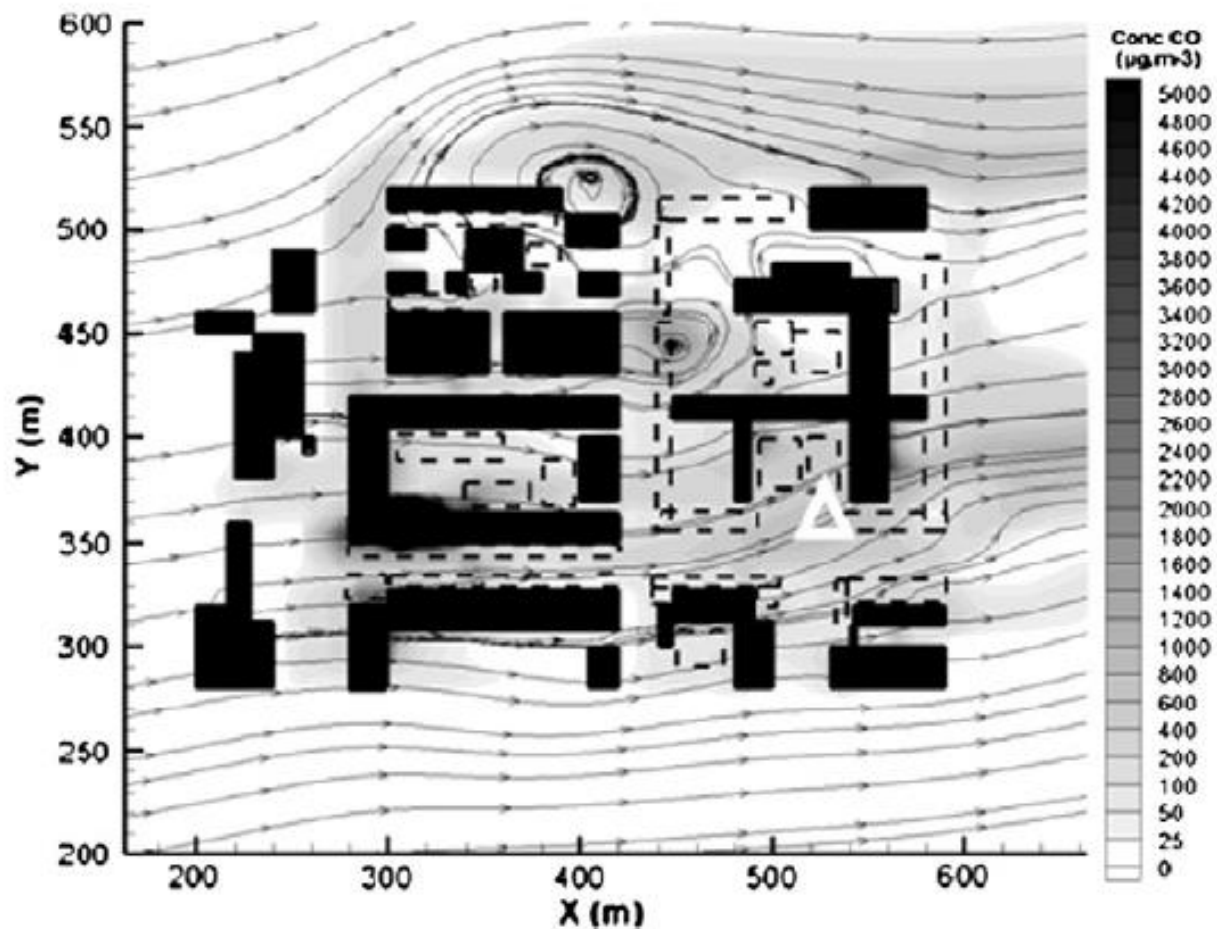


Figure 5-1 Modeling results showing the 3 m high horizontal streamlines and CO concentration field with effect of trees in Aveiro. Contours refer to the period between 10 and 11 a.m. Unfilled rectangles indicate trees blocks and the white triangle is the AQS location. (adapted from Amorim et al., 2013)

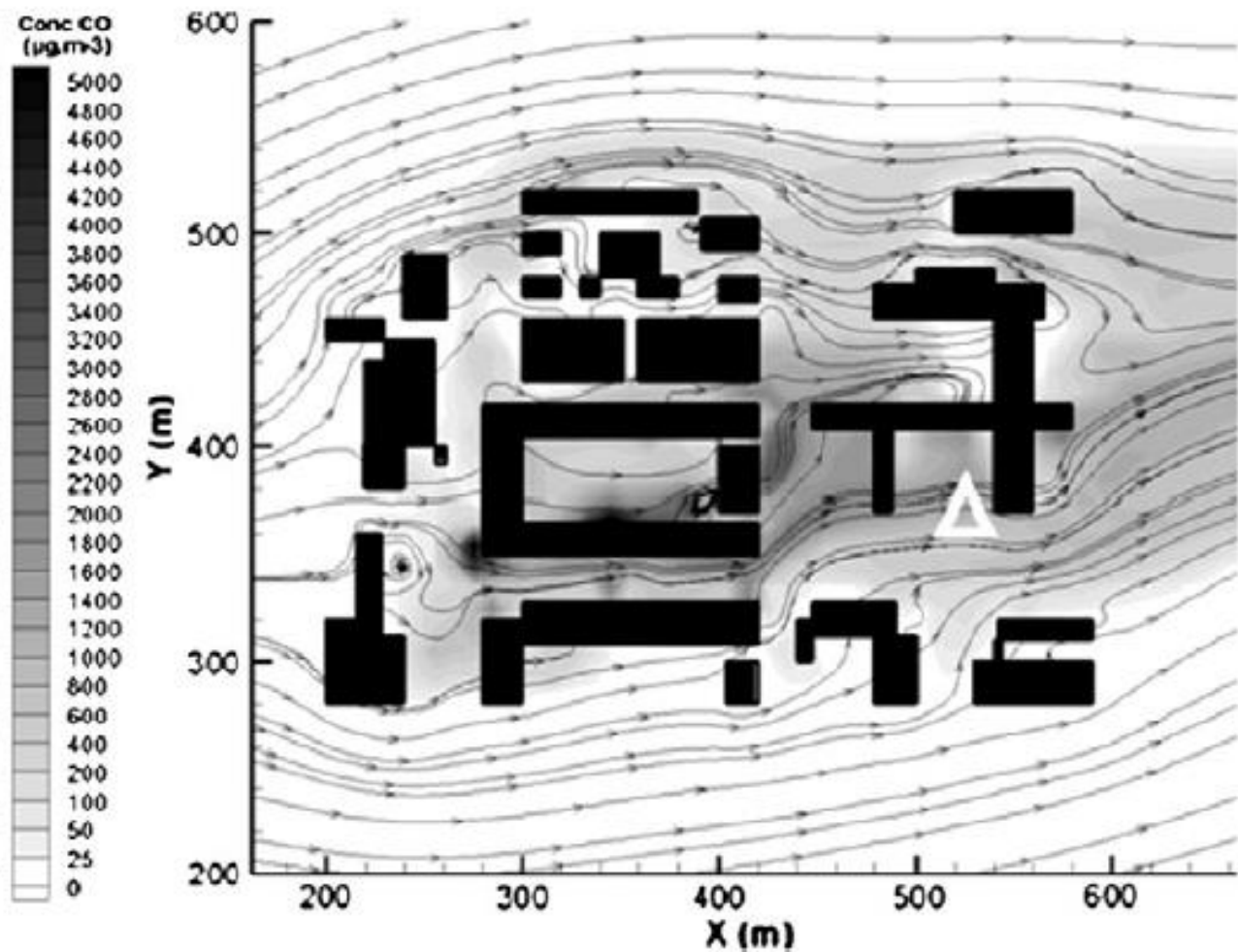


Figure 5-2 Modeling results showing the 3 m high horizontal streamlines and CO concentration field without the effect of trees in Aveiro. Contours refer to the period between 10 and 11 a.m. Unfilled rectangles indicate trees blocks and the white triangle is the AQS location. (adapted from Amorim et al., 2013)

Huang et al. simulated pollutant dispersion in the city of Kawasaki, Japan during the winter (Huang et al, 2008). A 400 meter by 400 meter area of Kawasaki was replicated in a 3-dimensional model. A RANS CFD model was compared to concentration measurements of NO and CO in Kawasaki at 13 different locations. In addition, the author applied a non-isothermal model and compared results to an isothermal model from the author's previous work. The non-isothermal model accounts for the solar radiation on roofs, walls, and the ground. Temperatures

were predicted based on the position of the sun, shading, and wind speed. The model accounted for conductive, convective, and radiative heat transfer. Weather measurements were collected for the Kawasaki area on a specific day and applied to the simulation, but a power law was assumed for the wind speed profile. Atmospheric stability was not addressed in this paper. Results were presented for five different day-time hours, but only two of the five time-snapshots are presented in graphical form in this paper at 9:00 and 11:00 o'clock. Figure 5-3 shows surface temperature (top) and NO concentration (bottom) at 9:00 o'clock. Likewise Figure 5-4 shows the surface temperature (top) and NO concentration (bottom) at 11:00 o'clock. The authors concluded that non-isothermal modeling of pollutant dispersion resulted in slightly lower pollutant concentrations when compared to isothermal modeling. This paper shows that isothermal assumptions may be a conservative assumption in the modeling of pollution dispersion in CFD models. This paper also shows that it is possible to simulate a large urban area in a CFD model.

The University of Applied Sciences Western Switzerland funded a project called the "Clean City." The main objective of this project is to reduce pollution concentration in cities by building placement and implementing roof structure to change the wind and increase pollution dispersion (Triscone et al., 2016). In this study, a scale model and a CFD model were built for the Paquis neighborhood in Geneva. Figure 5-5 shows the scale model and the emission of sulfur hexafluoride (SF_6). The CFD simulation was performed with a RANS model and the computations were performed with a cloud computing solution. The scale model was placed in a wind tunnel and multiple sources of pollutants were simulated by releasing SF_6 from streets and chimneys. These same sources were replicated in the CFD model and concentration measurements were collected at the same locations in both models. Figure 5-6 shows the

agreement of air velocity and dimensionless concentrations. The authors conclude that the CFD model replicates the behavior of both wind and dispersion, and that modeling results are in close agreement with wind tunnel measurements. This paper shows the possibility of replicating a city landscape with CFD modeling.

There are a number of other applications where CFD can be employed to model pollutant/contaminant dispersion. CFD models may be used to model acute hazards from accidental events, such as a chemical fire that produces toxic combustion products. These are typically used when there is complex geometry. Large scale weather may be modeled with CFD to simulate the impact of smoke from a large fire, like a forest fire. Another application is modeling specific weather conditions; for example, modeling pollution dispersion during an inversion.

While it is feasible to model pollution dispersion in urban areas with CFD, the applications are limited. CFD models must be validated for specific applications. These models are complex and the model inputs require a high level of specificity; thus validation is the preferred method of demonstrating “fit for purpose”. The application of CFD to large urban areas requires additional large-scale experiments, where extensive data is collected for both weather and pollutant concentrations. Based on recent research CFD models seem to be limited to domains that cover only a portion of a city. Increased efficiency will be required to model a large city (the full city, not a portion of a city) with a significant level of detail. Although, with current technologies Philips et al. was able to model a large urban canopy with the use of LES (Philips et al., 2013). Currently, CFD modeling of pollution dispersion in urban areas is relatively expensive because it requires expensive validation sets and intense computation.

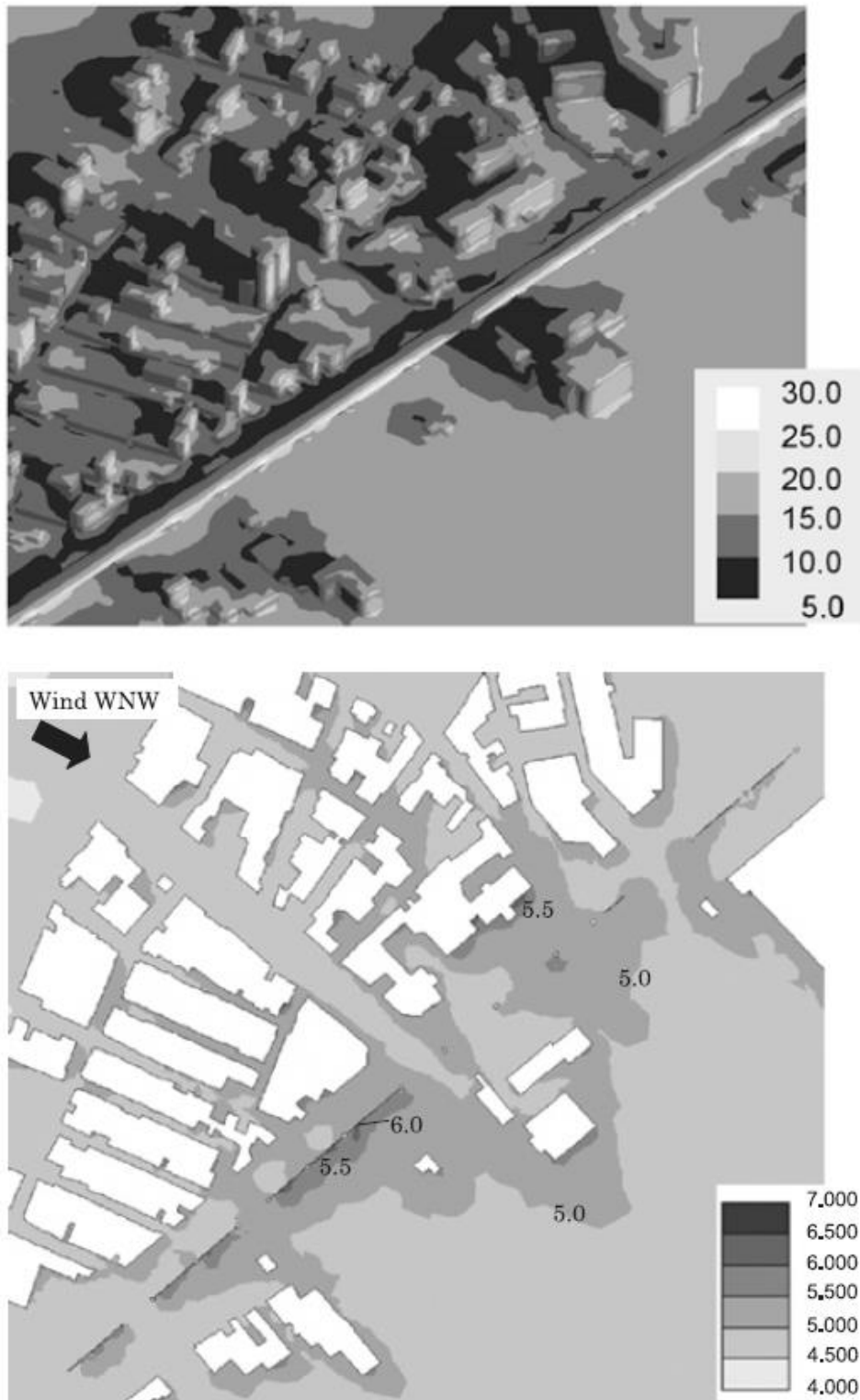


Figure 5-3 Top - Surface temperature in Celcius at 9:00 hours. Bottom - NO concentration (ppm) at 9:00 hours. (adapted from Huang et al., 2008)

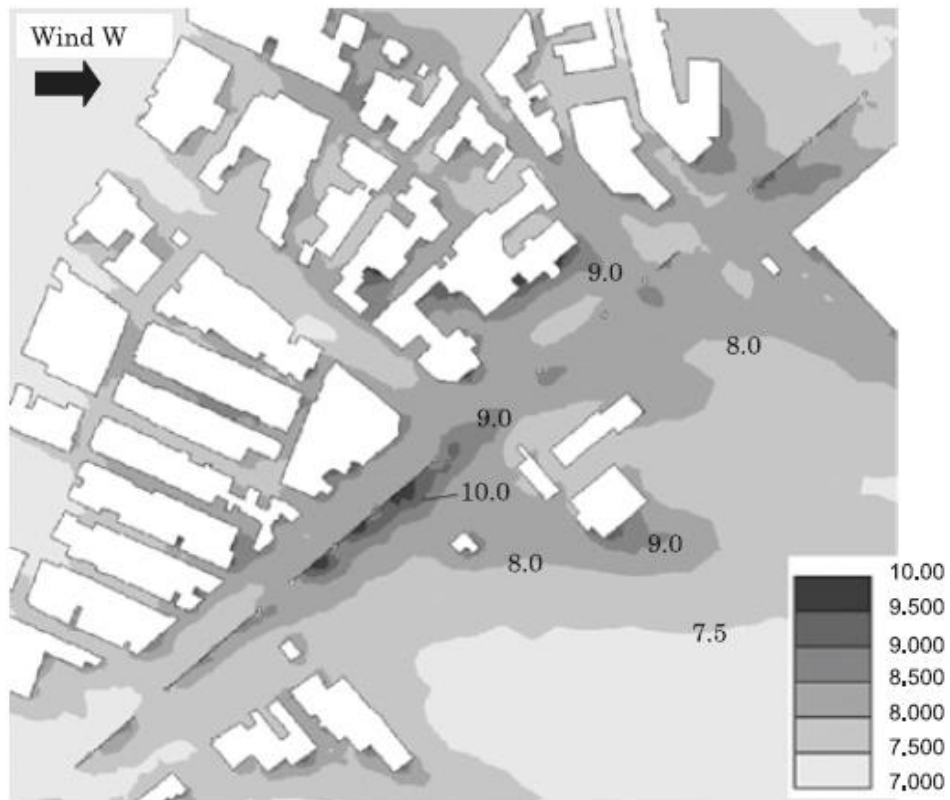
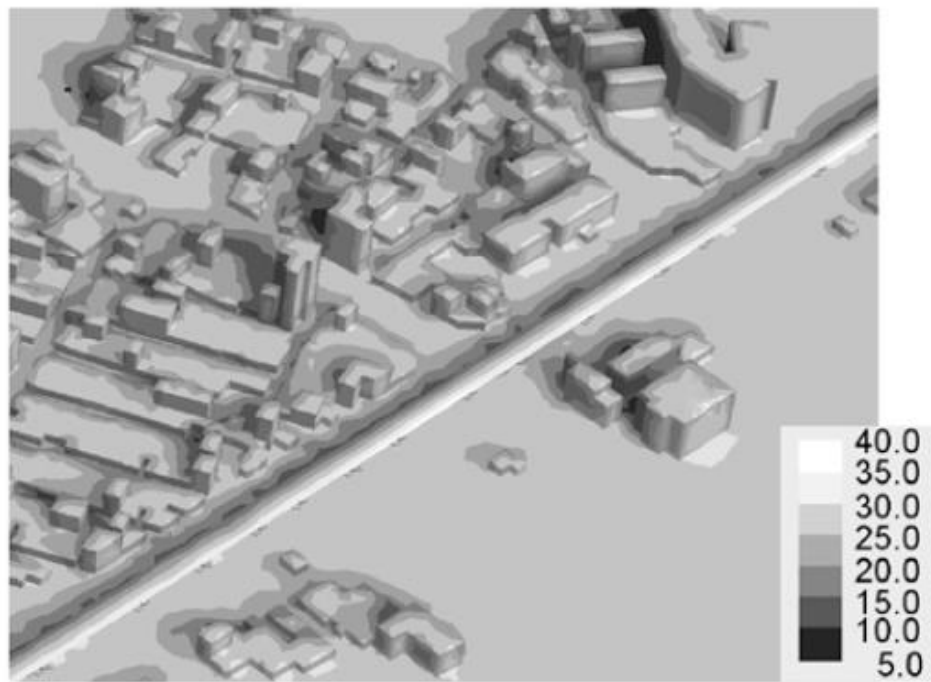


Figure 5-4 Top - Surface temperature in Celcius at 11:00 hours. Bottom - NO concentration (ppm) at 11:00 hours. (adapted from Huang et al., 2008)

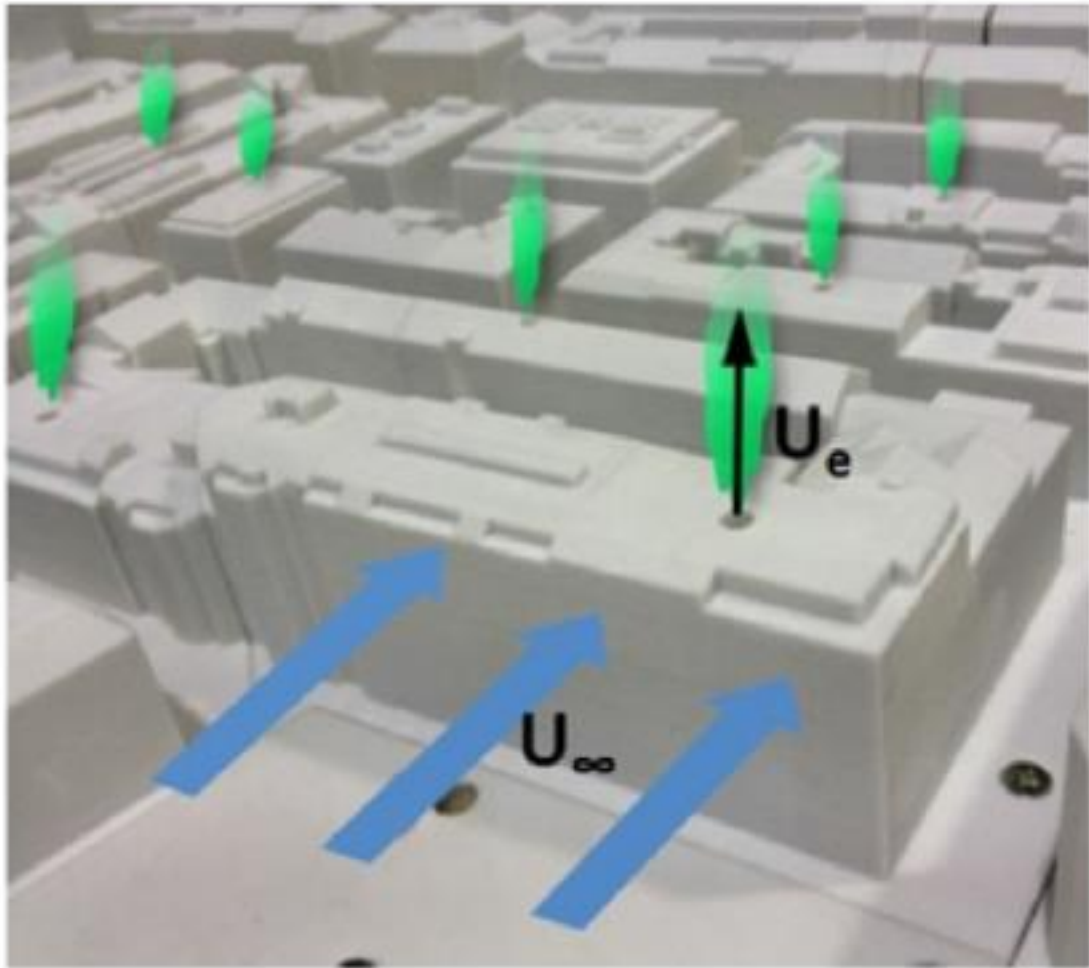


Figure 5-5 Physical scale model of the Pâquis city landscape, where the green indicates emission of SF6 and the blue arrows represent the air flow. (adapted from Triscone et al., 2016).

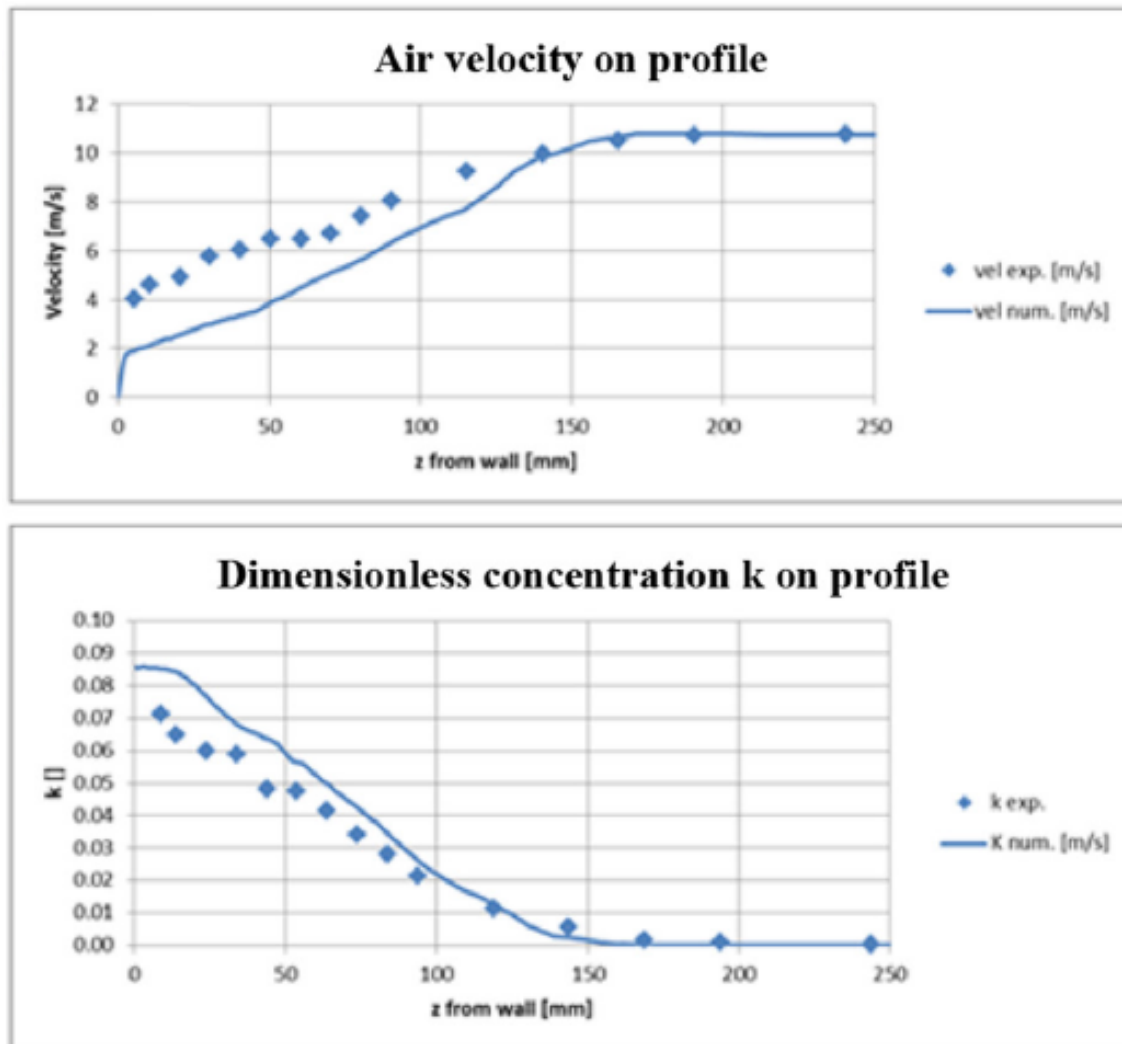


Figure 5-6 Top - wind speed as a function the height z . Bottom - measurements of dimensionless gas concentration. (adapted from Triscone et al., 2016).

Chapter 6 - Future Study

There are still many areas where further study could benefit the research into pollution modeling with CFD models. One area that is often ignored in the current research is weather conditions and model inputs relating to the weather. As presented earlier in Chapter 2, the wind speed profile and atmospheric stability are significant factors on dispersion in general. Another area that is often neglected in the current research is traffic interactions with the flow field. Other related topics that are not the main topic of this paper are: increasing the efficiency of CFD computation, meshes for 3-dimensional models, cluster computing with CFD solvers, and validating models.

There needs to be more sensitivity studies with the different CFD models to determine the level of impact the weather conditions have on the results. Many authors relied on simplified weather data, such as applying a single wind speed instead of a wind profile. Even when a wind profile was used, some authors based it solely on the wind speed measured at one elevation and assumed a profile function. More research is needed into the sensitivity of the models to different wind speed profiles. While some research has been reported (Basu and Porte-Agel, 2006; Koblitz et al., 2014; Pontiggia et al., 2009) atmospheric stability needs more attention in research. Atmospheric stability is a significant factor in determining dispersion. The complication with this is that atmospheric stability may need to be implemented differently for DNS, LES, RANS, and possibly specific CFD packages. In addition, inversions in the atmosphere can have a large impact on dispersion of pollutants. Depending on height of the inversion in relation to the city landscape or pollution sources, inversions may not be neglected when modeling pollutant dispersion in an urban landscape. Can inversions be forced into CFD

models or are temperature gradients important in developing accurate flow patterns. More research is needed into how inversions can be modeled and validated within CFD models.

Most of the research neglected the movement of traffic. More research is needed to determine if modeling a moving source of pollution can be simplified to a line source or another simplified pollution source. In addition, the movement of vehicles may increase the turbulence and mixing near the ground. Ignoring the increased dispersion that comes from vehicle movement results in higher pollutant concentrations, but it may be important in validating CFD models.

Chapter 7 - Conclusion

CFD provides an advanced tool to study pollutant dispersion in a city landscape. CFD allows inputs to be descriptive of weather conditions, but more research is needed to incorporate weather and atmospheric stability into CFD models. CFD modeling allows simulation of air quality for a complex geometry of a city landscape and different weather conditions to determine the behavior of pollution dispersion and pollutant concentration profile in a city. The recent research has shown that complex geometries, such as vegetation and city landscapes, can be simulated in CFD and produce reasonably close predictions compared to field measurements (Steffens et al., 2014; Huang et al, 2008; Triscone et al., 2016). In addition, an isothermal assumption for a city landscape has been shown to produce pollutant concentrations that are slightly higher than the non-isothermal case (Huang et al, 2008). More research is needed in the ongoing study of modeling pollution dispersion with CFD, for a large area and complex geometry, like a city landscape. CFD offers the possibility of identifying high concentrations of pollutants within an urban area and simulating pollutant concentrations for proposed changes to urban areas. This information could then be used to reduce the populations overall exposure to high concentrations of pollutants and ultimately reduce the negative health impacts caused by pollution.

References

- Amorim, J. H., Rodrigues, V., Tavares, R., Valente, J., & Borrego, C. (2013). CFD modelling of the aerodynamic effect of trees on urban air pollution dispersion. *Science of the Total Environment*, 461-462(C), 541-551.
- Basu, S., & Porte-Agel, F. (2006). Large-eddy simulation of stably stratified atmospheric boundary layer turbulence: A scale-dependent dynamic modeling approach. *Journal of the Atmospheric Sciences*; 63(8), 2074-2091.
- Batt, R., Gant, S., Jean-Marc Lacome, Truchot, B., & Tucker, H. (2018). CFD modelling of dispersion in neutrally and stably-stratified atmospheric boundary layers: Results for prairie grass and thorney island. *Int.J.of Environment and Pollution*, 63(1), 1-18.
- Chambers, S. D., Wang, F., Williams, A. G., Xiaodong, D., Zhang, H., Lonati, G., . . . Allegrini, I. (2015). Quantifying the influences of atmospheric stability on air pollution in Lanzhou, China, using a radon-based stability monitor. *Atmospheric Environment*, 107, 233-243.
- Chang, C., & Meroney, R. N. (2003). Concentration and flow distributions in urban street canyons: Wind tunnel and computational data. *Journal of Wind Engineering & Industrial Aerodynamics*, 91(9), 1141-1154.
- Coleman, Gary N. and Sandberg, Richard D. (2010) A primer on direct numerical simulation of turbulence - methods, procedures and guidelines (School of Engineering Sciences Aerospace Engineering AFM Reports, AFM 09/01a) Southampton, UK. University of Southampton.
- Finlayson-Pitts, B., & Pitts, Jr., J. (1999). *Chemistry of the Upper and Lower Atmosphere: Theory, Experiments, and Applications*. New York: Academic Press.
- Foken, T. (2008). *Micrometeorology*. Berlin: Springer-Verlag Berlin Heidelberg. Retrieved January 22, 2019 from <https://link-springer-com.er.lib.k-state.edu/book/10.1007%2F978-3-540-74666-9>
- Gatski, T., Hussaini, M., Lumley, T., & Lumley, John L. (1996). *Simulation and Modeling of Turbulent Flows*. (ICASE/LaRC series in computational science and engineering). New York: Oxford University Press.
- Huang, H., Ooka, R., Chen, H., Kato, S., Takahashi, T., & Watanabe, T. (2008). CFD analysis on traffic-induced air pollutant dispersion under non-isothermal condition in a complex urban area in winter. *Journal of Wind Engineering & Industrial Aerodynamics*, 96(10), 1774-1788.
- Koblitz, Bechmann, Berg, Sogachev, Sørensen, & Réthoré. (2014). Atmospheric stability and complex terrain: Comparing measurements and CFD. *Journal of Physics: Conference Series*, 555(1), 10.

- Krishna, I. V. M., Manickam, V., Shah, A., & Davergave, N. (2017). *Environmental management: Science and engineering for industry*. Oxford: Elsevier Science
- Kwak, K., Kim, K., Seung-Bok, L., Bae, G., Young-Il, M., Young, S., & Jong-Jin, B. (2018). On-Road Air Quality Associated with Traffic Composition and Street-Canyon Ventilation: Mobile Monitoring and CFD Modeling. *Atmosphere*, 9(3), 92.
- Launder, B. E., & Spalding, D. B. (1974). The numerical computation of turbulent flows. *Computer Methods in Applied Mechanics and Engineering*, 3(2), 269-289.
- Mavroidis, I., Andronopoulos, S., & Bartzis, J. G. (2012). Computational simulation of the residence of air pollutants in the wake of a 3-dimensional cubical building. the effect of atmospheric stability. *Atmospheric Environment*, 63, 189-202.
- NCEI (2019) - National Centers for Environmental Information. (n.d.). Retrieved January 19, 2019 from <https://www.ncdc.noaa.gov/crn/measurements.html>
- Pasquill, F., & Smith F. B. (1983). *Atmospheric diffusion* (3rd ed.). Chichester, West Sussex: Halsted Press.
- Philips, D., Rossi, R., & Iaccarino, G. (2013). Large-eddy simulation of passive scalar dispersion in an urban-like canopy. *Journal of Fluid Mechanics*, 723, 404-428.
- Pontiggia, M., Derudi, M., Busini, V., & Rota, R. (2009). Hazardous gas dispersion: A CFD model accounting for atmospheric stability classes. *Journal of Hazardous Materials*, 171(1), 739-747.
- Pope, C. (2007). Mortality Effects of Longer Term Exposures to Fine Particulate Air Pollution: Review of Recent Epidemiological Evidence. *Inhalation Toxicology*, 19(S1), 33-38.
- Rückerl, R., Schneider, A., Breitner, S., Cyrys, J., & Peters, A. (2011). Health effects of particulate air pollution: A review of epidemiological evidence. *Inhalation Toxicology*, 23(10), 555-592.
- Som, S., Senecal, P.K., Pomraning, E. (2012). Comparison of RANS and LES Turbulence Models against Constant Volume Diesel Experiments, presented at ILASS Americas 24th Annual Conference on Liquid Atomization and Spray Systems, San Antonio, TX, May 2012.
- Steffens, J., Heist, D., Perry, S., Isakov, V., Baldauf, R., & Zhang, K. (2014). Effects of roadway configurations on near-road air quality and the implications on roadway designs. *Atmospheric Environment*, 94, 74-85.
- Steffens, J., Heist, D., Perry, S., & Zhang, K. (2013). Modeling the effects of a solid barrier on pollutant dispersion under various atmospheric stability conditions. *Atmospheric Environment*, 69, 76-85.

- Steffens, J. T., Wang, Y. J., & Zhang, K. M. (2012). Exploration of effects of a vegetation barrier on particle size distributions in a near-road environment. *Atmospheric Environment*, 50, 120-128.
- Tabatabaian, M. (2015). *CFD module* Mercury Learning & Information. Retrieved from https://books.google.com/books?id=5Da_DgAAQBAJ
- Triscone, G., Abdennadher, N., Balistreri, C., Donzé, O., Greco, D., Haas, P., . . . Despot, F. (2016). Computational fluid dynamics as a tool to predict the air pollution dispersion in a neighborhood-a research project to improve the quality of life in cities. *International Journal of Sustainable Development and Planning*, 11(4), 546-557.
- United Nations. (16 May 2018). *68% of the world population projected to live in urban areas by 2050, says UN*. Retrieved from <https://www.un.org/development/desa/en/news/population/2018-revision-of-world-urbanization-prospects.html>
- WMO - World Meteorological Organization. (2017). Guide to meteorological instruments and methods of observation (2014 edition). Retrieved from https://library.wmo.int/doc_num.php?explnum_id=4147
- Wyngaard, J. (2010). *Turbulence in the atmosphere*. Cambridge, UK ; New York: Cambridge University Press.
- Zheng, Y., Miao, Y., Liu, S., Chen, B., Zheng, H., & Wang, S. (2015). Simulating Flow and Dispersion by Using WRF-CFD Coupled Model in a Built-Up Area of Shenyang, China. *Advances in Meteorology*, 2015, 15.